

Species Tag:	81001	Species Name:	Cl-35-NO2
Version:	1		Nitryl chloride,
Date:	May 1996		<sup>35</sup> Cl isotope
Contributor:	H. S. P. Müller		
Lines Listed:	3520	Q(300.0)=	87532.1324
Freq. (GHz) <	600	Q(225.0)=	55251.5340
Max. J:	80	Q(150.0)=	29375.3141
LOGSTR0=	-10.6	Q(75.00)=	10285.6424
LOGSTR1=	-7.3	Q(37.50)=	3637.3396
Isotope Corr.:	-0.122	Q(18.75)=	1287.8512
Egy. (cm <sup>-1</sup> ) >	0.0	Q(9.375)=	456.7436
$\mu_a$ =	$0.53 \pm 0.01$	A=	13290.137
$\mu_b$ =		B=	5175.4968
$\mu_c$ =		C=	3719.5377

The ground state microwave and millimeter wave data were taken from (1) T. Oka and Y. Morino, 1963, J. Mol. Spectrosc. **11**, 349; and (2) R. R. Filgueira, P. Forti, and G. Corbelli, 1975, J. Mol. Spectrosc. **57**, 97. Hyperfine splittings were not taken into account.

Also included in the fit are several infrared transitions: (3)  $\nu_4$  at 1684 cm<sup>-1</sup>, J. Orphal, M. Morillion-Chapey, and G. Guelachvili, 1994, J. Mol. Spectrosc. **165** 315; (4)  $\nu_1$  at 1282 and 2  $\nu_6$  at 1305 cm<sup>-1</sup> (Fermi resonance), J. Orphal, G. Guelachvili, and M. Morillion-Chapey, 1994, J. Mol. Spectrosc. **166** 280; (5)  $\nu_3$  at 370 cm<sup>-1</sup> and  $\nu_2$  at 793 cm<sup>-1</sup>, J. Orphal *et al.*, to be published.

The dipole moment is from D. F. Eagle, T. L. Weatherly, and Q. Williams, 1966, J. Chem. Phys. **44**, 847. It should be noted that a dipole moment of  $0.42 \pm 0.01$  D was reported by D. J. Millen and K. M. Sinnott, 1958, J. Chem. Soc., 350. This value is based on a much smaller data set and seems to be less reliable.

The partition function has been calculated up to  $J = 99$  because of the low rotational constant. The vibrational states used in the fit were also used in the calculation of the partition function. It should be noted that these are not all (low-lying) modes that occur.